

Replacement Pages for Claims 1-18

(CLEAN FORM)

Sub 2
1. A method for use in deriving fixed bond information, comprising:
analyzing a delocalized representation of a chemical structure;
identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;
evaluating at least a subset of the fixed bond representation candidates; and
selecting from among the plurality of fixed bond representation candidates based on the evaluation.

2. A system for use in deriving fixed bond information, comprising:
an analyzer analyzing a delocalized representation of a chemical structure;
an identifier identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;
an evaluator evaluating at least a subset of the fixed bond representation candidates; and
a selector electing from among the plurality of fixed bond representation candidates based on the evaluation.

3. Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive fixed bond information, the instructions causing the system to:
analyze a delocalized representation of a chemical structure;
identify, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;
evaluate at least a subset of the fixed bond representation candidates; and
select from among the plurality of fixed bond representation candidates based on the evaluation.

4. The method of claim 1, wherein at least a portion of the delocalized representation describes a monocyclic ring system.

5. The method of claim 1, wherein at least a portion of the delocalized representation describes a polycyclic ring system.

Sub 3

6. The method of claim 1, wherein at least a portion of the delocalized representation describes a ring system with a hetero substitution pattern.

7. The method of claim 1, wherein at least a portion of the delocalized representation describes a non-cyclic system.

SUB B2) 8. The method of claim 1, wherein at least a portion of the delocalized representation describes an incompletely cyclic system.

SUB C5) 9. The method of claim 1, further comprising:
including, in the produced fixed bond representation, a pair of opposite charges lacked by the delocalized representation.

10. The method of claim 1, further comprising:
including, in the produced fixed bond representation, a pair of radicals lacked by the delocalized representation.

SUB D1) 11. The method of claim 1, further comprising: -
queuing at least a subset of the candidates by priority.

12. The method of claim 1, further comprising:
using a precomputed table of atom valences as a function of element, charge, radical state, and number and distribution of bonds inside and outside of a delocalized region in the delocalized representation.

13. The method of claim 1, wherein the table includes an extensible component.

SUB B3) 14. The method of claim 1, wherein the table is extensible to apply to any chemical element.

SUB C18) 15. The method of claim 1, further comprising:
deriving electronic state and valence distributions information together with analyzing the delocalized representation.

16. The method of claim 1, further comprising:
determining whether it is practicable to produce a fixed bond representation of the chemical structure.

SUB D1) 17. The method of claim 1, further comprising:
determining whether it is possible to produce a fixed bond representation of the chemical structure that meets a set of radicals requirements.

18. The method of claim 1, further comprising:

2. determining whether it is possible to produce a fixed bond representation of the chemical structure that meets a set of charges requirements.
